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MEASUREMENT OF STACKING FAULT PROBABILITIES IN BULK SPECIMENS

H. M. Otte, D. O. Welch and G. F. Bolling

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# MEASUREMENT OF STACKING FAULT PROBABILITIES IN BULK SPECIMENS

H. M. Otte,\* D. O. Welch\* and G. F. Bolling\*\*

Recently Welch and Otte (1962) pointed out that residual elastic strains can affect measurements of the stacking fault probability,  $\alpha$ , in face-centered cubic metals. The purpose of this note is to consider one case in detail, where strains were not examined, and to draw attention to some precautions which must be taken in interpreting the measured shifts of X-ray reflections.

In the investigation of zone-refined lead by Bolling et al. (1961), bulk specimens were examined at 4.2°K and 77°K. The deformation at temperature was performed by scraping the surface of the specimens (gouging). Even though the nature and distribution of any residual lattice strains would be quite complex and certainly would depend on the exact manner of deformation, it is possible that a residual strain predominantly of one sign was left in the specimens. This strain would lead to a shift in the position of each X-ray reflecting depending on the scattering angle and the elastic constants. Since lead is more anisotropic elastically than the other f.c.c. metals, it turns out that the effect of residual lattice strains is relatively most important for lead.

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When residual elastic strain and faulting are both considered, the following equation should be used to calculate  $\alpha$ ,

$$\delta \Delta 2\theta_{p-q} = K_{p-q} \sigma + H_{p-q} \alpha. \quad (1)$$

Here,  $\delta \Delta 2\theta_{p-q}$  represents the change in separation between the  $p^{\text{th}}$  and  $q^{\text{th}}$  X-ray reflections;  $H_{p-q}$  as defined by Wagner (1957), are coefficients relation the change in separation to the faulting probability; and  $K_{p-q}$  are coefficients relating the change to the residual stress,  $\sigma$ . The constants  $K_{p-q}$  are derived simply from the differential form of Bragg's law and the definition  $\epsilon_p = K_p \sigma$ ; i.e.,

$$K_{p-q} = -\frac{180}{\pi} 2 (K_p \tan \theta_p - K_q \tan \theta_q) \quad (2)$$

The moduli  $K_r$  can be calculated from the elastic constants under the two simplified extremes of constant strain or constant stress existing throughout the specimen. Greenough (1952) gives the equations for the strain  $\epsilon_{hk\ell}$  in the  $hk\ell$  direction and it follows that

$$\left. \begin{aligned} K_r [\epsilon = \text{const.}] &= \frac{-(C_{11} + 4C_{12} - 2C_{44})}{2(C_{11} + 2C_{12})(C_{11} - C_{12} + 3C_{44})} \\ \text{and } K_r [\sigma = \text{const.}] &= S_{12} + \frac{(S_{11} - S_{12} - \frac{1}{2} S_{44})(h^2 k^2 + k^2 \ell^2 + \ell^2 h^2)}{(h^2 + k^2 + \ell^2)^2} \end{aligned} \right\} (3)$$

where  $C_{ij}$  and  $S_{ij}$  are the elastic constants and  $r = h^2 + k^2 + l^2$ . In most cases, however, the best agreement with observation is not obtained under these extreme assumptions; better agreement is obtained if the actual residual strain distribution is considered to be somewhere between the limits of isotropic stress and isotropic strain, (Greenough, 1952; Welch and Otte, 1962). The  $K_r$  for this assumed situation is chosen here to be the average of the values of  $K_r$  in equation (3).

The stress and the faulting probability can both be derived from equations (1) if the change in separation between two pairs of X-ray reflections are measured. For the zone-refined lead such changes were measured at 4.2°K; the reflections involved were the 111, 200, and 220, lines 3, 4, and 8 respectively (Bolling et alia, 1961). The value of the coefficients to be used for lead examined with  $\text{CuK}\alpha$  radiation ( $\lambda = 1.5418\text{\AA}$ ) are given in Table I.

Calculated values for the stacking fault probability and the residual stress are given in Table II. The usual assumption of zero residual strain ( $K=0$ ), gives values of  $\alpha$  very close to those derived at the assumed extreme of isotropic strain. However, the stress values for both seem unreasonable;  $\sigma = 0$ , or -6 and -8  $\text{Kg/mm}^2$ . At the other assumed extreme, of isotropic stress, the value of  $\alpha$  has been appreciably diminished and it is also somewhat diminished under the assumed, mean case. The four values of stress from -2 to -4  $\text{Kg/mm}^2$  fall below the stress at the beginning of necking observed in single crystals of lead deformed in tension at 4.2°K, (Bolling et

al., 1962); and because it is not unusual to obtain high values of stress in compression these values must be considered reasonable. Since the deformation was by gouging, any residual strain in the direction of the surface normal would most likely have been predominantly positive, reflecting a transverse compressive stress in the deformed surface. The calculated stresses are therefore of the expected sign.

In the investigation at 4.2°K, specimens of aluminum and a Cu-30Zn alloy were also deformed by gouging. Unfortunately, the results from neither material can be used to clarify the effects of residual strain. Aluminum is quite isotropic elastically and there would have been little effect. The brass on the other hand is anisotropic elastically, but it faults profusely and the changes in line separation due to the deformation faults would most likely have masked any effects of residual strain due to the anisotropy.

Other experiments (Welch and Otte, 1962) have shown that residual elastic strains can make a significant contribution to the peak shifts in an anisotropic f.c.c. alloy. It can also be concluded here that the contribution is measurable in lead if the averaging assumption holds true, and quite significant, if the extreme of isotropic stress holds true. In the work performed by Bolling et al. (1961) the  $\delta\Delta_{4-3}^{2\theta}$  was primarily relied upon; it is however advisable in this sort of experiment to examine as many X-ray peaks as possible in order to take account of the contribution due to residual strains. Finally, the precaution should be added that, even though the use of filings provides an averaging that should eliminate the extreme of



isotropic stress, it is not clear that the effects of residual elastic strain have been experimentally shown to be negligible.

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TABLE I

Coefficients and Data Used in Equations (1) for Lead at 4.2°K \*

<u>Quantity</u>	<u>4-3</u>	<u>8-4</u>	<u>Units</u>
First cold work $\delta \Delta 2\theta$	$-0.03_0(\pm 0.01)$	$0.02_3(\pm 0.02)$	$^\circ(2\theta)$
Second cold work $\delta \Delta 2\theta$	$-0.04_8(\pm 0.01)$	$0.03_8(\pm 0.02)$	$^\circ(2\theta)$
$H_{p-q}$	-3.7	4.5**	$^\circ(2\theta)$
$K_{p-q}$ Constant strain	0.00053	0.00181	$^\circ(2\theta)\text{mm}^2/\text{Kg}$
$K_{p-q}$ Constant stress	0.00930	-0.00445	"
$K_{p-q}$ Mean Case Average of above	0.00491	-0.00132	"

\* The data is taken from Bolling et al (1961). A lattice constant  $a_0 = 4.916 \text{ \AA}$  and the elastic constants for lead at 4.2°K, given by Waldorf (1960), were used.

\*\* The value of  $H_{8-4}$  was incorrectly given by Bolling et al (1961) as 7.8, but was not significantly used.

TABLE II

Calculated Values of Stacking Fault Probability and Residual Stress- First Cold Work -

Quantity	Assumptions			
	$\epsilon = 0$	$\epsilon = \text{constant}$	$\sigma = \text{constant}$	mean Case
$\alpha$	0.008 0.005 } 0.006 <sub>5</sub>	0.007	0.003	0.004
$\sigma$ , Kg/mm <sup>2</sup>	0	-6	-2	-3

- Second Cold Work -

$\alpha$	0.013 0.008 } 0.010 <sub>5</sub>	0.012	0.005	0.007
$\sigma$ , Kg/mm <sup>2</sup>	0	-8	-3	-4

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